

MO 6: Atomic clusters (with MO)

Time: Monday 17:00–19:00

Location: C/Foyer

MO 6.1 Mon 17:00 C/Foyer

Radio-frequency buncher for core-level photoelectron spectroscopy of metal clusters at FLASH — ●FRANKLIN MARTINEZ, PATRICE OELSSNER, MICHAEL KÖTHER, JOSEF TIGGESBÄUMKER, and KARL-HEINZ MEIWES-BROER — Universität Rostock, Institut für Physik, 18055 Rostock

XUV radiation of high brilliance from the free electron laser facility FLASH (Hamburg) allows to access electronic core levels of free metallic clusters by photo-electron spectroscopy (PES). Recent experiments on lead cluster anions revealed a systematic shift of 5d and of 4f level energies as a function of cluster size. For small clusters, a variation of the electron binding energy from the metallic sphere model due to reduced core-hole screening is observed [1,2]. However, with decreasing cluster size and also with increasing photon energies, the photoionization cross sections decrease rapidly, thus limiting the photo-electron yield. To increase the target density of size-selected clusters, and hence the electron yield, a new apparatus with a linear radiofrequency ion trap is currently under construction. Perspectively, the ion trap is to be combined with a radio-frequency ion buncher to increase the cluster density in the laser interaction region even further. With this setup many-electron dynamics due to x-ray photon absorption and highlycorrelated phenomena on ultrashort timescales in clusters will be addressed in future experiments. This contribution reports about design and simulations of the rf-buncher. The work is funded by the bmbf (FSP302), and supported by the DFG (SFB 652). [1] V. Senz et al., PRL 102, 138303 (2009). [2] J. Bahn et al., NJP 14, 075008 (2012).

MO 6.2 Mon 17:00 C/Foyer

Investigation of a ring ion trap for the production of multiply-charged cluster anions — ●STEFAN KNAUER, GERRIT MARX, and LUTZ SCHWEIKHARD — Institut für Physik, Universität Greifswald, Felix-Hausdorff-Str. 6, 17489 Greifswald

A multipole ring trap was built for systematic studies of cluster anions. The Coulomb barrier and electron binding energies of multiply-charged metal clusters are experimentally mostly uninvestigated. Because polyanionic metal-clusters do not exist in nature, they have to be produced in laboratories by cluster electron collision. This can be achieved by combinations of cluster sources and ion traps [1]. A method to investigate the Coulomb barrier is the production of negative charge states with precise electron energies. To do so, one needs a field free region for the cluster-electron interaction where, simultaneously, the cluster ions are trapped. For this purpose a multipole ring electrode trap [2] was built. The experiment consists of a magnetron sputter source [3], a quadrupole bender, the ring electrode trap and a section for time-of-flight mass spectrometry (ToF MS). The sputter source is used to produce singly-charged negative metal clusters, which are guided into the trap. Cooled cluster ions can gain multiple charge states by cluster-electron collisions. For those collisions the cluster and electrons have to interact in a field free region, which a ring-electrode trap provides. In a next step, the experiment should provide defined charge states for laser interaction experiments. The contribution will discuss the principle and design of the ring electrode trap, preliminaryion-confinement tests and corresponding mass spectra.

MO 6.3 Mon 17:00 C/Foyer

Linear Paul-trap for core-level photoelectron spectroscopy of Metal Clusters at FLASH — ●MICHAEL KÖTHER, FRANKLIN MARTINEZ, PATRICE OELSSNER, JOSEF TIGGESBÄUMKER, and KARL-HEINZ MEIWES-BROER — Universität Rostock, Institut für Physik, 18055 Rostock

Previous photoelectron spectroscopy experiments at the free electron laser in Hamburg (FLASH) have shown distinct changes in the binding energy of lead 5d and 4f levels as a function of cluster size[1,2]. With higher photon energies available it is now possible to excite even deeper core electrons. On the other hand photoionization cross sections decrease rapidly. For compensation higher target densities are necessary and will be achieved by a new setup currently under construction. The main changes include a cryogenic, linear Paultrap and a radio frequency ion buncher. In the trap, cluster ions from a continuous source are cooled and accumulated, thus approaching a structural

ground state, before pulsed extraction into the FEL interaction region. This contribution reports about simulations and first test runs of the Paultrap. The work is funded by the BMBF FSP 302, and supported by the DFG (SFB 652). [1] V. Senz et al., Phys.Rev.Lett.,102, 138303 (2009). [2] J. Bahn et al., New J. Phys., 14, 075008 (2012).

MO 6.4 Mon 17:00 C/Foyer

Electron re-localization dynamics in Xenon clusters under intense XUV pump-probe excitation — ●MATHIAS ARBEITER, CHRISTIAN PELTZ, and THOMAS FENNEL — University of Rostock, Germany

Intense and temporally structured X-ray - light fields enable the controlled generation of strongly coupled nonequilibrium cluster nanoplasma. Sub-picosecond relaxation dynamics within the cluster are revealed via the delay dependent charge states as demonstrated in recent femtosecond soft x-ray pump-probe experiments [1]. Here we report a scheme based on local electron single-particle energy spectra that enables microscopic tracing of the underlying electron-relocalization processes in molecular dynamics simulations up to the strong-coupling regime [2]. We show that recombination dynamics strongly depend on temperature and density of the system leading to a rapidly converging electron relocalization within a few picoseconds and most efficient recombination in the cluster core. A systematic pump-probe analysis reveals that electron re-localization provides a fingerprint of electron cooling and nanoplasma rarefaction through cluster expansion and yield delay-dependent ion charge states in good agreement with experiments[1]. The applied analysis is not restricted to soft x-ray excitation of clusters but essential also for the infrared regime and high harmonic light sources.

MO 6.5 Mon 17:00 C/Foyer

Microscopic description of single-shot diffractive imaging of atomic clusters — ●KATHARINA SANDER, CHRISTIAN PELTZ, and THOMAS FENNEL — Institute of Physics, University of Rostock

The availability of intense femtosecond laser pulses in the XUV and soft x-ray spectral range from free-electron lasers has made it possible to investigate the structure and dynamics of nanosystems via single-shot diffractive imaging experiments, as recently demonstrated with single clusters [1]. To study the linear light scattering in clusters theoretically we employ the discrete dipole approximation (DDA) [2]. The DDA method relies on a dyadic Greens function approach and allows to model arbitrarily shaped targets down to the atomic level. We propose a modified complex mixing scheme to increase convergence of the iterative DDA model. As a first application, we examine the possibility of imaging the recently predicted IR induced nonlinear internal plasma waves in clusters [3]. Our analysis supports that distinct features of the sub-fs dynamics can be extracted from time-resolved scattering pictures. Second, we investigate the scattering of strongly absorbing silver clusters. A comparison with experimental results highlights the necessity to include absorption, which is neglected in the regularly applied treatment of x-ray scattering (Born approximation). Finally, we analyze the limits for the applicability of the single-frequency approximation in the modelling of scattering images.

[1] T. Gorkhover *et al.*, Phys. Rev. Lett. **108**, 245005, (2012)[2] E. M. Purcell *et al.*, Astrophys. J. **186**, 705-714, (1973)[3] C. Varin *et al.*, Phys. Rev. Lett. **108**, 175007, (2012)

MO 6.6 Mon 17:00 C/Foyer

Time-resolved X-ray Imaging of Anisotropic Nanoplasma Expansion — ●CHRISTIAN PELTZ¹, CHARLES VARIN², THOMAS BRABEC², and THOMAS FENNEL¹ — ¹Institute of Physics, University of Rostock, Germany — ²Department of Physics and Centre for Photonics Research, University of Ottawa, Canada

We investigate the time-dependent evolution of laser-heated R = 25 nm solid-density hydrogen clusters via coherent diffractive imaging for an infrared pump / x-ray probe scenario. Our microscopic particle-in-cell analysis provides a full self-consistent electromagnetic description of both the droplet ionization and expansion induced by the intense few-cycle pump pulse as well as the elastic and inelastic light scattering by the x-ray probe in the expanding nano-plasma [1]. Our analysis reveals that continuous ion ablation on the cluster surface generates an anisotropic nanoplasma expansion that can be accurately described

by a simple self-similar radial density profile. Its time evolution can be reconstructed precisely by fitting the time-resolved scattering images using a simplified scattering model in Born approximation. Our findings suggest, that time-resolved diffractive imaging experiments on nano-droplets will provide unprecedented insights into the physics of ion expansion and surface ablation in laser-driven plasmas [2].

[1] C. Varin, C. Peltz, T. Brabec and T. Fennel, *Phys. Rev. Lett.* **108**, 175007 (2012)

[2] C. Peltz, C. Varin, T. Brabec and T. Fennel, *Phys. Rev. Lett.* **113**, 133401 (2014)

MO 6.7 Mon 17:00 C/Foyer

Commissioning the Microfocus Optics for the CAMP Chamber at FLASH — ●JAN P. MÜLLER¹, BENJAMIN ERK², REBECCA BOLL², CEDRIC BOMME², EVGENY SAVELYEV², GÜNTER BRENNER², SIARHEI DZIARZHYTSKI², BARBARA KEITEL², MARION KUHLMANN², ELKE PLÖNJES², KAI TIEDKE², ROLF TREUSCH², MARIO SAUPPE¹, ANGAD SWIDERSKI², LARS GUMPRECHT³, THOMAS TILP³, FRANK SIEWERT⁴, THOMAS ZESCHKE⁴, DANIEL ROLLES², and THOMAS MÖLLER¹ — ¹TU Berlin/ IOAP, AG M^oller, 10623 Berlin — ²DESY, 22607 Hamburg — ³CFEL, 22607 Hamburg — ⁴HZB, 12489 Berlin

Free electron lasers provide a high photon flux combined with ultrashort pulse durations. A tightly focussed radiation beam enables to study atoms, molecules, clusters and particles with nonlinear effects, particularly light scattering. A focus smaller than $8 \times 9 \mu\text{m}^2$ has been reached by a newly set-up Kirkpatrick-Baez optics at the BL1 of FLASH. In combination with the permanently installed CAMP chamber [1], a multi-purpose instrument for electron and ion spectroscopy, pump-probe, and imaging experiments, it founds the base for user-experiments at high light intensities in a versatile and well-proven experimental chamber. In a first experiment very high charge states of

ions from a rare gas target could be generated.

[1] L. Strüder et al., Large-format, high-speed, x-ray pnCCDs combined with electron and ion imaging spectrometers in a multipurpose chamber for experiments at 4th gen. light sources, *Nucl. Instr. and Meth. in Phys. Res. A* **614**, 483–496 (2010)

MO 6.8 Mon 17:00 C/Foyer

First-principles simulation of alkali-doped liquid helium at zero temperature — ●STEFAN HEMPEL, YAROSLAV LUTSYSHYN, and DIETER BAUER — Institut für Physik, Universität Rostock, 18051 Rostock, Germany

Alkali-doped helium droplets reveal unexpected physical features [1,2] and present testing grounds for first-principles quantum many-body methods [3]. In particular, multiple Mg dopants are known to form metastable structures in helium droplets [2]. We use first-principles projector Monte Carlo methods to study how the presence of the alkali atoms affects the surrounding superfluid. We will report the implications for the interpretation of the metastable structures of Mg atoms in the droplets.

[1] M. Mudrich, F. Stienkemeier, *Int. Rev. Phys. Chem.* **33**, 301–339, (2014); J. Reho, U. Merker, M. R. Radcliff, K. K. Lehmann, G. Scoles, *J. Chem. Phys.* **112**, 8409 (2000).

[2] A. Przystawik, S. Göde, T. Döppner, J. Tiggesbäumker, and K.-H. Meiwes-Broer, *Phys. Rev. A* **78**, 021202(R) (2008); S Göde, R Irsig, J Tiggesbäumker and K-H Meiwes-Broer, *New J. Phys.* **15**, 015026 (2013).

[3] R. Rodríguez-Cantano, T. González-Lezana, P. Villarreal, D. López-Durán, F. A. Gianturco, G. Delgado-Barrio, *Int. J. Quantum Chem.* **114**, 1318 (2014); A. Nakayama, K. Yamashita, *J. Chem. Phys.* **114**, 780 (2001).